NUMERICAL 3D MODEL FOR THERMAL INTEGRATION OF 20W METHANOL REFORMER

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1. ABSTRACT

Collaborative U.S. Army and U.S. Department of Energy efforts have developed advanced methanol reforming capabilities to enhance production of hydrogen for soldier portable fuel cell systems. Application of advanced numerical techniques combined with empirical data from iterative breadboard measurements has provided the US Army with an 8.5x2x0.8 cm 20W methanol reformer for Future Force Warrior and Future Combat Systems.

2. INTRODUCTION

Fuel cell technology development is being pursued around the world to provide electric power in many potential applications in the military and commercial sector. These applications range in size from milli-watts to mega-watts. Major investments are being made to develop fuel cell systems for mobile use and for stand-by power applications. Near-term Future Combat Systems (FCS) mobile platforms, Future Force Warrior and commercial automotive use are predominantly focused on the Proton Exchange Membrane (PEM) fuel cell technology. For the stand-by/residential power applications, investments are being made in both PEM and Solid Oxide Fuel Cell (SOFC) technologies. However, the closest to market for the military, commercial and residential/standby power applications is judged to be PEM technology.

The Army's one fuel forward is the ultimate goal, and the techniques, reported herein, are applicable that that application as well. However, due to the challenges resulting from sulfur in diesel fuel/JP8, methanol is the near term solution, and hence, was the source of the hydrogen in this case. Presently, in the stand-by power case, natural gas or propane is the most likely source of hydrogen. In both cases, high energy/power density and efficient fuel processors/reformers are key technological barriers to actual military and commercial use of fuel cell systems. The effort to develop these processors/reformers represents a major percentage of the military and commercial investment in technology development.

3. NUMERICAL CODE DESCRIPTION

One of the U.S. Army RDECOM efforts to advance small/compact and efficient fuel processors was the development of a 20 W methanol reformer by Pacific Northwest National Laboratory (PNNL). Due to energy/power density and system operation requirements, thermal integration was a key part of the reformer development. To assist in this effort, the Army developed a Computational Fluid Dynamics (CFD) model of the prototype designs as they were developed. A conservative, finite volume formulation was used to solve the transient equations for the conservation of mass, momentum and energy on a structured multi-block domain. An implicit formulation was used with a second order hybrid upwind differencing scheme, to represent the advective terms, and a second order Crank-Nicolson scheme to represent the diffusive terms. Navier-Stokes equations were used with the laminar flow accounted for in the diffusive terms since the micro-channel Reynolds Number was in the range of 90. Velocity – pressure coupling, for continuity, was achieved using the SIMPLEC algorithm (Van Doormal and Raithly,1984) for collocated (non-staggered) grids, which was developed on the basis of the SIMPLE algorithm (Patankar and Spaulding, 1972) for staggered grids. Rhie Chow Interpolation (Rhie and Chow, 1983) was used to smooth out checkerboard oscillations in pressure and velocity and yield an error on the order of the 4^{th} derivative.

The modeling effort was a semi-empirical effort where PNNL instrumented bread-board components to supply the Army with experimental data such as micro-combustor heat generation, exhaust gas temperatures, exhaust gas flowrate, fuel and oxygen inlet flowrate and temperature, micro-reactor flows and micro-reactor heat absorption from the endothermic reactions. Also, geometry and material information was provided by PNNL to the Army.

A segregated solver was used to converge upon the velocity profiles in the micro-channels during steady state operation. Instrumentation requirements to measure velocity and temperature profiles in micro-channels would have been extensive, time consuming and

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expensive, hence, CFD modeling offered several advantages to such measurements. Once the velocity profiles were converged, the energy equation was included to account for conduction and convection in steady state and transient operation.

Good agreement was found in those locations which were accessible to instrumentation. The model was used to determine the best prototype designs that would transfer heat from the micro-combustor to the micro-reactor and from the micro-combustor to the vaporizers to yield the correct temperatures for the associated reactions and phase changes while producing axial micro-reactor temperature profiles that were advantageous.

4. REFORMER TRANSIENTS

Transient predictions were conducted for the purpose of minimizing the reformer startup time, which is the time required for convection and conduction from the micro-combustor to 1) heat up the "pre-heating sections" that preheat the incoming methanol and air, 2) heat up the vaporizer sections leading to the micro-combustor and the reformer and 3) heat up the micro-reactor channel and associated catalyst. Prior to that time, batteries or other power sources will be required to maintain operation. Reformer designs that reduce startup periods, also reduce the associated battery size and weight requirements.

Solutions of the time-dependent, conservation of mass, three dimensional momentum, and energy were required to predict the three dimensional velocity and temperature gradients. To obtain those gradients conjugate heat transfer was applied. This work was conducted to predict the speed and manner of the transient startup response leading to steady state operation. This is important because start up times of 15 minutes or more are common and some kind of power source is required during that period to preheat and vaporize fuel to the micro-combustor. This is also includes the time required to heat the micro-reactor section with heat convected and conducted from the micro-combustor exhaust gas. Similar conditions occur during periods of low hydrogen demand if the micro-combustor heat output is controlled dynamically with demand to conserve fuel and provide power for longer mission durations. Upon reformer startup, internal flow developed to the steady state condition in a short period compared to energy. This period was a small fraction of the time required for the energy equation to progress to a steady state. This allowed for a large reduction in computational requirements by allowing the hydrodynamic solution to progress to steady state with small time steps, while omitting the energy equation. The solution to the hydrodynamic equations were then held constant and the energy equation was solved at a relatively large time step due to the thermal capacitance of the stainless steel solid material. This eliminated the need to solve the hydrodynamic equations and the energy equation simultaneously and avoid the inefficiency caused by solving the hydrodynamic equations and energy equation at the small time steps.

5. TRANSIENT RESULTS

Figure 1 is a top view of the breadboard 20W reformer. An advantage of the semi-empirical technique reported here is that the breadboard allowed accurate measurement of 1) mass flow rates, 2) heat absorbed due to the endothermic reactions in the reformer, 3) heat absorbed due to phase change in the vaporizer section and 4) the heat output due to the exothermic reaction in the micro-combustor. An additional advantage is that the three dimensional temperature gradients across the meso-channels and across the stainless steel were predicted, rather than measured, which if possible, would have been difficult and expensive to conduct non-intrusively. A disadvantage of this technique is that the measured heat gains and sinks from the endothermic and exothermic reactions are assigned as uniform along these sections in the numerical code.

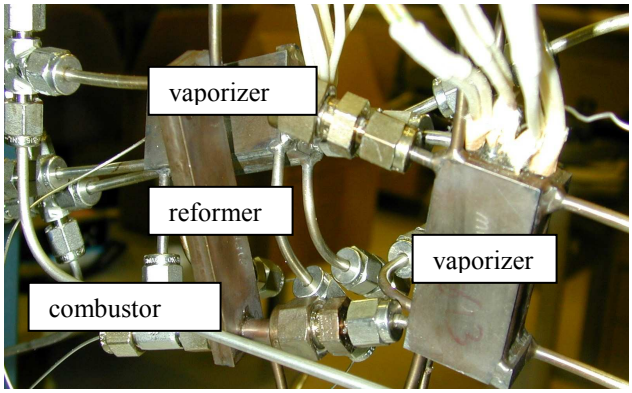

Figure 1: 20W Methanol Reformer Breadboard.

The overall advantage of this type of modeling is that a virtual integrated reformer system can be designed and optimized for thermal integration during the breadboard tests using a blend of numerical and empirical parameters. Figure 2 is an example of one of the virtual reformer systems that was used to guide the iterative design of the actual reformer system. Figures 3, 4 and 5 show predicted, transient temperature gradients in one of the virtual prototype reformer systems. The red shades represent the micro-combustor and micro-combustor exhaust gases exiting the immediate proximity of the micro-combustor. The left side of the geometry is the preheater section for the micro-combustor. Conduction to this preheater section, is a determining factor to startup times.

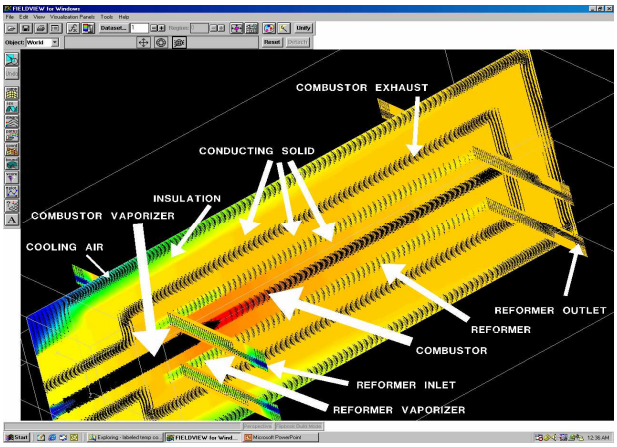

Figure 2: Color shaded map of temperature distributions on the center cross section of a virtual integrated reformer operating at near steady state..

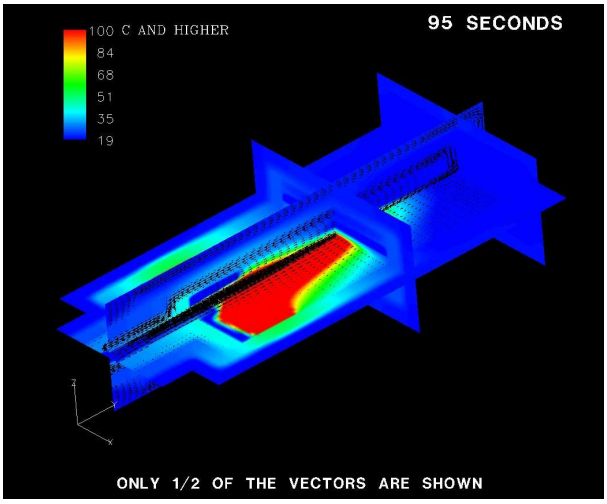

Figure 3: Color shaded temperature distribution at reformer system midplanes at time = 95 seconds.

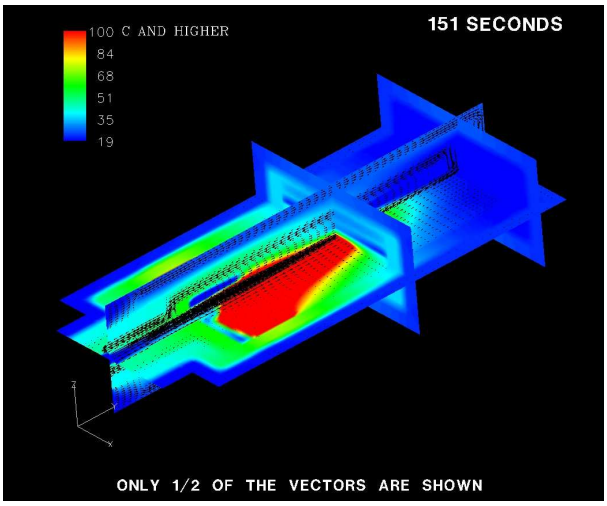

Figure 4: Color shaded temperature distribution at reformer system midplanes at time = 151 seconds.

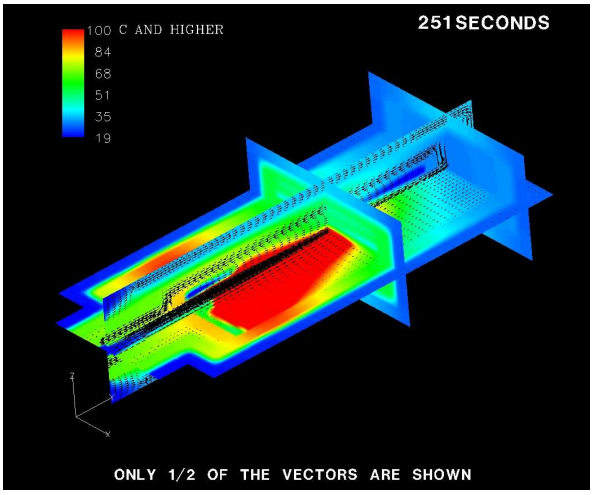

Figure 5: Color shaded temperature distribution at reformer system midplanes at time = 251 seconds.

In summary, the three dimensional numerical model predicted spatial and temporal temperature distributions that helped to guide and optimize the iterative design process that lead to the final design.

6. IMPACT OF NUMERICAL MODEL

The exterior geometry of the resulting integrated reformer system is shown in Figure 6. The performance specification for hydrogen production was exceeded by 33%, from 15W to 20W. The final dimensions were 8.5x2x0.8 cm. Additionally, the insulative effect of enveloping the reformer system in Aerogel, for integration into a reformed fuel cell system, was included and is shown on the perimeter of the simulations displayed in Figures 2 through 5.

Figure 6: Exterior geometry of integrated reformer system.

7. SUMMARY AND FUTURE EXPERIMENTS

Application of advanced numerical techniques combined with empirical data from iterative breadboard measurements has provided the US Army with a 8.5x2x0.8 cm 20W methanol reformer for Future Force Warrior and Future Combat Systems. The performance specification for hydrogen production was exceeded by 33%, from 15W to 20W.

Now that numerical techniques have been successfully applied to enhance designs at an integrated system level, plans are being made to apply these techniques to address shortcomings inside individual sections, like the micro-reactor section.

8. REFERENCES

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